Some mathematical aspects of topological materials (New topics of transformation groups)

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Some mathematical aspects of topological materials

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Abstract

I shall present a concise summary of some mathematical aspects of topological materials for topologists without much background of physics. I shall summarize how physical properties of a crystal yield some vector bundle on the Brillouin torus, which is constructed from the crystal, by which, some important physical quantities are translated into (equivariant) homotopy theoretical invariants of these vector bundles. For instance, the classical TKNN formula states that the Hall conductivity, induced by the Lorenz force, is quntized by the 1^{st} Chern class of the corresponding vector bundle. We shall also report a recent remark of Gomi-De Nittis, which claims the Fu-Kane-Mele $\mathbb{Z}_2$-invariant of the topological insulators (quantum spin Hall effect) is the FKMM invariant of the corresponding "Quaternionic"vector bundle.

1 Introduction

The theory of Topological matters studies the homotopy theory of matters, i.e. physical properties stable under small perturbations. The essential ideas may be summarized as follows:

- Symmetry of a crystalline solid defines its Brillouin torus.
- Physical properties of a crystalline solid, described by some "energy" i.e. some Schrödinger operator on some Hilbert space ,
  $\Longrightarrow$ (equivarint) vector bundle on the Brillouin torus.
- Physical invariants may be expressed by some homotopy theoretical invariants of (equivariant) vector bundles.

In this summary, I concisely review some mathematical aspects of the topological materials by explaining these points. My presentation follows [C, DN-G]. For the transparency and the brevity, I have omitted the bulk-edge correspondence, for which, the readers are referred to [GP].

2 Brillouin torus

We start with a mathematical "definition"of an our physical objective:

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crystal $\mathcal{C}$: the locations of atoms in $\mathbb{R}^d$ $(d = 2, 3)$, which is invariant by discrete translations T_γ of vectors γ in *a chosen* Bravais lattice $\Gamma \cong \mathbb{Z}^d (\subseteq \mathbb{R}^d)$.

Now, to construct the Brillouin torus, we must work in the dual space, in which we define the dual lattice of the Bravais lattice Γ:

reciprocal lattice $\Gamma^\star := \{G \in \mathbb{R}^d \mid \forall \gamma \in \Gamma,\ G \cdot \gamma \in 2\pi\mathbf{Z}\}$.

Then, we can define the requisited Brillouin torus by quotienting out the dual space $\mathbb{R}^d$ by this reciprocal lattice $\Gamma^\star$:

d-dimensional Brillouin torus BZ $:= \mathbf{R}^d/\Gamma^\star$.

3 (equivarint) vector bundle on the Brillouin torus

In order to quantum mechanically represent physical states on the crystal $\mathcal{C}$ caused by a finite number of internal degrees of freedom of atoms, e.g. the spin of electrons, we prepare a finite-dimensional complex vector space V equipped with a scalar product $\langle -, - \rangle_V$. For simplicity, we shall consider the tight-binding model, in which electronic wave functions are restricted to the crystal $\mathcal{C}$ (with canonical extensions to elsewhere). Then the physical states of an electron in this crystal $\mathcal{C}$ are represented by:

Hilbert space of crystalline states $\mathbf{H} = \ell^2(\mathcal{C}, \mathbf{V})$ **:** the space of V-valued square-summable functions on $\mathcal{C}$ with the scalar product

$$\langle \psi | \chi \rangle = \sum_{x \in \mathcal{C}} \langle \psi(x) | \chi(x) \rangle_V .$$

$\mathbf{H}$ reflects the symmetry of the crystal $\mathcal{C}$, through:

T_γ, the translation of states $\psi \in \mathbf{H}$ by $\gamma \in \Gamma$: the unitary operator T_γ on $\mathbf{H}$ such that

$$T_\gamma \psi(x) = \psi(x - \gamma), \quad x \in \mathcal{C}.$$

Then an energy eigenstate of an electron corresponds to:

Bloch function $\psi(x) \in \mathbf{H}$ with quasi-momentum $k \in \mathbb{R}^d/\Gamma^\star = \mathbf{BZ}$: Eigenfunctions of all unitary operators T_γ $(\gamma \in \Gamma)$

$$\begin{aligned} \Longrightarrow\ & \exists k \in \mathbb{R}^d/\Gamma^\star = \mathrm{BZ} \text{ s.t.} \\ & T_\gamma \psi(x)\,(:= \psi(x - \gamma)) = e^{ik\cdot\gamma}\psi(x), \quad \forall x \in \mathcal{C}, \forall \gamma \in \Gamma. \end{aligned}$$

From these, we now have a tractible finite dimensional vector space $\mathcal{H}_k$ for each quasi-momentum $k \in \mathbb{R}^d/\Gamma^\star = \mathrm{BZ}$:

finite dim'ℓ Hilbert space $\mathcal{H}_k$ with $\dim(\mathcal{H}_k) = |\mathcal{C}/\Gamma| \times \dim(\mathbf{V})$**:**

- made of Bloch functions on $\mathcal{C}$ with quasi-momentum $k \in \mathbb{R}^d/\Gamma^\star = \mathrm{BZ}$;

- equipped with the scalar product

$$\langle \psi_k | \chi_k \rangle_k = \sum_{x \in \mathcal{C}/\Gamma} \overline{\psi}_k(x) \chi_k(x).$$

$\mathcal{H}$, the Bloch bundle on the Brillouin torus $\mathbb{R}^d/\Gamma^\star = \mathbf{BZ}$:

- $\dim(\mathcal{H}_k) = |\mathcal{C}/\Gamma| \times \dim(\mathbf{V})$ dim'ℓ complex v.b.;
- whose fiber at $k \in \mathbb{R}^d/\Gamma^\star = \mathrm{BZ}$ is $\mathcal{H}_k$.
- with Hermitian structure.
- The Fourier transform $\psi(x) \mapsto \widehat{\psi_k}$ induces a norm preseving identification:

$$\mathbf{H} := \ell^2(\mathcal{C}, \mathbf{V}) \cong L^2(\mathrm{BZ}, \mathcal{H})$$

$$\psi(x) \mapsto \left(k \mapsto \widehat{\psi}_k(x) = \sum_{\gamma \in \Gamma} \mathrm{e}^{-\mathrm{i}k\cdot\gamma} \psi(x-\gamma) \in \mathcal{H}_k \right)$$

$$\psi(x) := \frac{\int_{\mathrm{BZ}} \widehat{\psi_k}(x) dk}{|\mathrm{BZ}| := \int_{\mathrm{BZ}} dk} \leftarrow \left(k \mapsto \widehat{\psi}_k(x) \right)$$

- In fact...

  Bad News: The vector bundle $\mathcal{H} \to \mathrm{BZ}$ is trivial.

We are still in such boring mathematical situation, because we have not reflected the nature of the electronic phase in the physical side yet. We must take into account the "energy" (Hamiltonian) of the physical property:

periodic Hamiltonian H: The invariance of $\mathcal{C}$ by T_γ's forces the Hamiltonian H periodic w.r.t. Γ.

$\Longrightarrow$ H and T_γ's commute

$\Longrightarrow$ Can simultaneously diagonalize H and T_γ's!

Bloch Hamiltonian H_k: the Hamiltonian action$H$ restricts to the finite dim'ℓ vector space $\mathcal{H}_k$ for each $k \in BZ$:

$$H : \mathcal{H} \to \mathcal{H}$$

$$\Longrightarrow H_k : \mathcal{H}_k \to \mathcal{H}_k,$$

where H_k may be expressed by a Hermitian matrix with spectra (eigenvalues)

$$\mathrm{Spec}\, H_k = \left\{ (E_k)_1 \leqq (E_k)_1 \leqq \cdots \leqq (E_k)_{|\mathcal{C}/\Gamma|\cdot\dim\mathbf{V}} \right\}$$

To construct a tractible subvector bundle of $\mathcal{H}$, which reflects rich physical phase of the crystal $\mathcal{C}$, we impose the following assumption:

Insulator assumption: $\exists$ Fermi energy ϵ_F , s.t.

$$\forall k \in \mathrm{BZ},\ \epsilon_F \notin \mathrm{Spec}\, H_k \qquad (\textit{ i.e. an insulator. })$$

$\mathcal{E}_k$: The subspace of $\mathcal{H}_k$, spanned by the eigenspaces whose eigenvalues are stricktly smaller than the Fermi energy ϵ_F,

$\mathcal{E}$: the valence-band subbundle of the Bloch bundle $\mathcal{H}$, whose fiber at $k \in \mathrm{BZ}$ is above $\mathcal{E}_k$.
This is the vector bundle we really wish to study!

4 Quantum Hall effect and 1^{st} Chern class c_1

Consider a plate (in the xy-plane) crystalline insulator at the absolute temperature $T = 0$:

$$\begin{cases} B_z & := \text{the strength of the magnet field applied in} \\ & \quad \text{the } z\text{-direction, which we fix and make inexplicit.} \\ E_y & := \text{the strength of the electronic field applied in} \\ & \quad \text{the } z\text{-direction, which we explicitly vary.} \end{cases}$$

Then the Lorenz force

$$\vec{F} = q\left(\vec{E} + \vec{v} \times \vec{B}\right)$$

is responsible for

$$j_x := \text{electronic currency in the } x\text{-durection.}$$

$\langle j_x \rangle$: the expected value of j_x w.r.t. the Fermi-Direc distribution

$$f(E,T) = \frac{1}{e^{\beta(E-\epsilon_F)+1} + 1} \quad \left(\beta = \frac{1}{k_B T}\right)$$

at the absolute temperature $T = 0$.

The Hall conductivity $\sigma_{xy} := \frac{\langle j_x \rangle}{E_y}$: Klaus von Klitzing experimentally discovered the integer Quantum Hall effect:

$$\sigma_{xy} = \frac{e^2}{h} \times (\text{integer})$$

Here, set $V = \mathbb{C}$ and $H = \frac{(-i\hbar\vec{\nabla})^2}{2m} + V(\mathbf{r})$, then the 1^{st} Chern class $c_1(\mathcal{E})$ of the valence-band subbundle $\mathcal{E}$ is shown to be responsible for this phenomenon:

Thouless-Kohmoto-Nightingale-den Nijs, Nakano (Kubo), Berry, Simons..

$$\begin{cases} \sigma_{xy} & = -\frac{e^2}{h} c_1(\mathcal{E}) \\ c_1(\mathcal{E}) & \in H^2(\mathrm{BZ}; \mathbb{Z}) = \mathbb{Z} \end{cases}$$

For more details, the reder is referred to [C].

5 FKMM invariant of Quaternionic vector bundles

Here, we take into account the special relativity and work with the Dirac equation

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = H\psi(\vec{x}, t)$$

$$H = c\vec{\alpha} \cdot (-i\hbar\vec{\nabla}) + \beta mc^2,$$

where

$$\vec{\alpha} = \left(\begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{pmatrix} \begin{pmatrix} & & & -i \\ & & i & \\ & -i & & \\ i & & & \end{pmatrix} \begin{pmatrix} & & 1 & \\ & & & -1 \\ 1 & & & \\ & -1 & & \end{pmatrix} \right), \beta = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix},$$

and the wave function is the 4 component Dirac spinor

$$\Psi(\vec{x}, t) = \begin{pmatrix} \psi_1(\vec{x}, t) \\ \psi_2(\vec{x}, t) \\ \psi_3(\vec{x}, t) \\ \psi_4(\vec{x}, t) \end{pmatrix}.$$

However, instead of the Dirac Hamiltonian

$$H = c\vec{\alpha} \cdot (-i\hbar\vec{\nabla}) + \beta mc^2$$

we work with **spin-orbit interaction Hamiltonian:**

$$H_{SO} := -\frac{e}{2m^2c^2} \frac{1}{r} \frac{d\phi}{dr} \mathbf{S} \cdot \mathbf{L},$$

where,

$$\mathbf{S} := \frac{1}{2}\hbar\vec{\sigma}, \quad \text{spin angular momentum operator},$$
$$\mathbf{L} := \mathbf{r} \times \mathbf{p}, \quad \text{orbit angular momentum operator},$$

and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is given by **Pauli matrices**

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Thus, in this case, we set $V = \mathbb{C}^4, H = H_{SO}$, but...

Bad News: The nontriviality of the valence-band Bloch bundle $\mathcal{E}$ in this case is elusive.

Good News: In this case, the time-reversal symmetry of the system makes the valence-band Bloch bundle "equivariant." This extra "equivariant"structure gives the valence-band Bloch bundle more chance of becoming nontrivial, at least "equivariantly".

Actually, for the spin-orbit interaction Hamiltonian

$$\begin{aligned} H_{SO} &= -\frac{e}{2m^2c^2} \frac{1}{r} \frac{d\phi}{dr} \mathbf{S} \cdot \mathbf{L} \\ &= -\frac{e}{2m^2c^2} \frac{1}{r} \frac{d\phi}{dr} \left(\frac{1}{2}\hbar\vec{\sigma}\right) \cdot (\mathbf{r} \times \mathbf{p}) \\ &= -\frac{e\hbar}{4m^2c^2} \frac{1}{r} \frac{d\phi}{dr} \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \cdot (\mathbf{r} \times \mathbf{p}), \end{aligned}$$

the time-reversal symmetry operator Θ becomes

$$\Theta = -i\sigma_2 K, \quad (K \text{ is the complex conjugate operator})$$

$$\Longrightarrow \begin{cases} [\Theta, H_{SO}] & = 0 \\ \Theta : \mathcal{H}_k & \to \mathcal{H}_{-k}, \ (k \in \mathrm{BZ}) \\ \Theta^2 & = -I_{\mathcal{H}}. \end{cases}$$

$\Longrightarrow$ Θ endows the block bundle $\mathcal{H}$ with

a "Quaternionic" vector bundle structure.

Here, a complex vector bundle $\pi : E \to X$ over a $\mathbb{Z}/2$-space $\tau : X \to X$ ($\tau^2 = I_X$) with a complex anti-linear lift $\tau_E : E \to E$:

$$\tau_E(\alpha v + \beta w) = \overline{\alpha}\tau_E(v) + \overline{\beta}\tau_E(w)$$

$$\tau \circ \pi = \pi \circ \tau_E$$

is called a

$$\begin{cases} \underline{\underline{\text{"Real" vector bundle}}} \\ \underline{\underline{\text{"Quaternionic" vector bundle}}} \end{cases}$$

if

$$\begin{cases} \tau_E^2 & = 1 \\ \tau_E^2 & = -1 \end{cases}$$

Now, De Nittis-Gomi [DN-G] proved the following translation of some important physical invariants of topological insulators to some mathematical invariants:

De Nittis-Gomi

Fu-Kane-Mele $\mathbb{Z}_2$-invariant of the topological insulators (quantum spin Hall effect) is the FKMM invariant of the "Quaternionic" vector bundle.

For the Fu-Kane-Mele $\mathbb{Z}_2$-invariant, see [FK, FKM, C]; for the FKMM invariant, see [DN-G, FKMM]; and for the proof of this theorem of De Nittis-Gomi, consult the original proof of [DN-G].

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